

# Temperature-Dependent Frequency Shifts in Collective Excitations of a Bose-Einstein Condensate

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## Abstract

By including the contribution of the thermal cloud to the Lagrangian of the condensate of a Bose gas, we extend the time-dependent variational method at zero temperature to study temperature-dependent low collective excitation modes. A Gaussian trial wave function of the condensate and a static distribution density of the thermal cloud are used, and analytical expressions for temperature-dependent excitation frequencies obtained. Theoretical results are compared with measurements in the JILA and MIT experiments.

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With the development of techniques to trap and cool atoms, Bose-Einstein condensation (BEC) has been observed directly in dilute atomic vapors [1–3]. The new experimental achievements have stimulated great interest in the theoretical study of inhomogeneous Bose gases. The collective excitations of trapped Bose gases, which describe their dynamics and transport properties, have been a focus of recent experimental and theoretical studies. Low-lying collective excitations over a range of temperatures [4–7] and higher-lying modes [8] have been measured in recent experiments.

In the regime with no detectable non-condensate fraction, theoretical predictions based on a mean-field description of weakly interacting bosons at zero temperature are in excellent agreement with experimental data [9–11]. At zero temperature, a Bose-Einstein condensate is described by the nonlinear Schrödinger equation (NLSE), i.e. the Gross-Pitaevskii equation [12],

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + U(\mathbf{r})\psi + \frac{4\pi\hbar^2 a}{m} |\psi|^2 \psi, \quad (1)$$

where  $m$  is the atomic mass,  $U(\mathbf{r})$  the trapping potential, and  $a$  the  $S$ -wave scattering length. Characterizing the evolution of the macroscopic wave function  $\psi$  of the condensate, this nonlinear equation provides a fundamental means for studying the ground state, dynamical behavior and collective excitations of the condensate. The validity of the Gross-Pitaevskii equation in describing the evolution of the condensate wave function has been verified by the quantitative comparison of theoretical predictions with experimental observations.

The Gross-Pitaevskii equation (1) has been solved by means of a time-dependent variational technique to obtain the low energy excitations of a trapped Bose gas for both positive and negative scattering lengths [13]. By taking a proper trial function of a fixed shape with some free time-dependent parameters, a variational technique based on Ritz's optimization procedure leads to a set of Newton-like ordinary differential equations of the second order for these parameters which characterize the solution to the NLSE. Avoiding expensive numerical simulations, this method affords analytical approximations which moreover provide a clear physical picture of the problem.

For a dilute Bose gas trapped in a harmonic potential, with a Gaussian function taken as the natural trial wave function for low energy states, expressions for frequencies of the collective modes in a 3D anisotropic trap have been obtained [13]. In the large particle number limit, the expressions contain the spectrum derived by Stringari [10] based on the Thomas-Fermi approximation, where the interatomic and trap interactions are dominant and the kinetic energy term is negligible.

The finite-temperature excitation spectrum has also been measured in the experiments of Refs. [6] and [7]. The spectrum has been studied by means of the Popov version of the Hartree-Fock Bogoliubov approximation [14,15] and by a two-fluid hydrodynamic approximation [16,17]. However, the finite temperature behavior of the spectrum observed in experiments has not been fully understood. In this paper, we extend the variational method at zero temperature to finite temperature where the thermal cloud exists. At a finite temperature, the thermal cloud provides an additional background field exerting on the condensate atoms, besides the mean-field interaction among them. The motion of the condensate can still be described by the nonlinear Schrödinger equation with the mean-field modified to include the effect of the thermal cloud. The evolution equation for the condensate may be derived from a variational principle to minimize the action of the corresponding Lagrangian density  $\mathcal{L}$ .

Let us consider a sample of Bosons confined in a  $d$ -dimensional harmonic potential

$$U(\mathbf{r}) = \frac{1}{2} \sum_{i=1}^d m\omega_i^2 x_i^2, \quad (2)$$

where  $\mathbf{r} = (x_1, x_2, \dots, x_d)$ . As shown in the recent experiment [7], we may neglect the mode coupling between the condensate and the thermal cloud. In this simplification, we assume the static thermal cloud density distribution to be

$$\rho_n(\mathbf{r}) = R(T) \exp[-U(\mathbf{r})/kT], \quad (3)$$

where  $R(T)$  is the normalization factor. The condensate moves in the combined field of the external trapping potential and the mean-field potential due to both the condensate and the

static thermal cloud. The Lagrangian density corresponding to the NLSE with the thermal cloud effect included can be written as

$$\mathcal{L} = \frac{i}{2}\hbar\left(\psi\frac{\partial\psi^*}{\partial t} - \psi^*\frac{\partial\psi}{\partial t}\right) + \frac{\hbar^2}{2m}|\nabla\psi|^2 + U(\mathbf{r})|\psi|^2 + \frac{2\pi a\hbar^2}{m}|\psi|^4 + \frac{4\pi\hbar^2 a}{m}\rho_n(\mathbf{r})|\psi(\mathbf{r})|^2 \quad (4)$$

where the asterisk denotes a complex conjugate. The normalization condition for the macroscopic wave function  $\psi(\mathbf{r})$  is

$$\int d\mathbf{r}|\psi|^2 = N_0,$$

where  $N_0$  is the number of the condensate atoms. The thermal cloud density normalizes according to

$$\int d\mathbf{r}\rho_n(\mathbf{r}) = N_n,$$

where  $N_n$  is the number of atoms in the thermal cloud. The last term in (4) comes from the interaction between the condensate and the thermal cloud [18].

Following Ref. [13], we consider the Gaussian trial function

$$\psi(\mathbf{r}, t) = A(t) \prod_i^d \exp\left\{-\frac{x_i^2}{2w_i(t)^2} + ix_i^2\beta_i(t)\right\}, \quad (5)$$

where, by setting the Gaussian distribution centered at the origin, we have ignored the irrelevant motion of the center of the condensate. The variational parameters are the amplitude  $A$ , width  $w_i$  and  $\beta_i$  relating to the curvature. All these parameters are real time-dependent functions, characterizing the macroscopic wave function of the condensate. Inserting the trial wave function into the Lagrangian density (4) and integrating over the coordinates, we obtain the Lagrangian

$$L(t) = \langle \mathcal{L} \rangle = \int_{-\infty}^{\infty} \mathcal{L} d\mathbf{r} \quad (6)$$

$$\begin{aligned} &= \sum_i^d N_0 \left( \frac{1}{4}m\omega_i^2 w_i(t)^2 + \frac{\hbar^2}{4mw_i(t)^2} + \frac{\hbar^2 w_i(t)^2 \beta_i(t)^2}{m} + \frac{1}{2}w_i(t)^2 \beta'_i(t) \right) \\ &\quad + \frac{2\pi N_0^2 a \hbar^2}{m} \prod_i^d \frac{1}{\sqrt{2\pi} w_i(t)} + \frac{4\pi N_0 N_n a \hbar^2}{m} \prod_i^d \sqrt{\frac{m\omega_i^2}{\pi kT}} \Big/ \sqrt{\frac{m\omega_i^2}{kT} w_i(t)^2 + 2}, \end{aligned} \quad (7)$$

where we have used the equation of particle number conservation

$$A(t) = N_0 \prod_i^d \frac{1}{\sqrt{\pi} w_i(t)}.$$

The last term in (7) is the contribution of the interaction between the condensate and the thermal cloud.

By minimizing the action corresponding to the Lagrangian with respect to the parameters, we can derive the ordinary equations describing the evolution of the parameters. The widths of the condensate satisfy the following equation:

$$w_i''(t) + \omega_i^2[1 - f(T)]w_i(t) = \frac{\hbar^2}{m^2 w_i(t)^3} + \frac{4\pi N_0 a \hbar^2}{m^2 w_i(t)} \prod_j^d \frac{1}{\sqrt{2\pi} w_j(t)}, \quad (8)$$

where, compared with the case of zero temperature, the thermal cloud contributes an extra term proportional to

$$f(T) = \frac{8\pi^2 N_n a \hbar^2}{m^2} \left( \frac{m}{2\pi kT} \right)^{\frac{d}{2}+1} \prod_{j=1}^d \omega_j.$$

In the derivation we have used the fact that the widths of the condensate are much smaller than those of the thermal cloud, i.e.  $m\omega_i^2 w_i(t)^2 \ll kT$ . If we regard the widths  $(w_1, w_2, \dots, w_d)$  as the coordinates of a fictitious particle, Eq. (8) is just Newton's equations of motion for the particle in the effective potential

$$V_{\text{eff}} = \frac{1}{2} \sum_{i=1}^d \left[ \omega_i^2 (1 - f(T)) w_i^2 + \frac{\hbar^2}{m^2 w_i^2} \right] + \frac{4\pi N_0 a \hbar^2}{m^2} \prod_i^d \frac{1}{\sqrt{2\pi} w_i}, \quad (9)$$

where the  $w_i^{-2}$  term corresponds to the kinetic energy of the condensate, the  $f(T)$  term to the contribution from the interaction between the condensate and the thermal cloud, and the last  $a$ -dependent term comes from the interatomic interaction of the condensate atoms.

After finding the widths, the curvature parameters  $\beta_i(t)$  can be obtained through the following equation derived from the variation principle

$$\beta_i(t) = \frac{mw'_i(t)}{2\hbar w_i(t)}. \quad (10)$$

Once the widths of the condensate are known, the rest of the parameters can be calculated, and the evolution of the Gaussian atomic cloud of the condensate can then be completely characterized. The whole problem of solving the NLSE reduces to that of solving the system of ordinary differential equations (8).

As a special case, we first consider a two-dimension isotropic trap. For the ‘breath’ mode with a radial symmetry, Eq. (8) reduces to

$$w''(t) + \omega^2(1 - f_2(T))w(t) = \frac{\hbar^2}{m^2 w(t)^3} + \frac{2N_0 a \hbar^2}{m^2 w(t)^3}, \quad (11)$$

where, for  $d = 2$ ,

$$f(T) = f_2(T) = 8\pi^2 N_n a \hbar^2 (\omega/2\pi kT)^2.$$

After introducing the new dimensionless constant  $p = 1 + 2N_0 a \hbar^2 / m^2$  and new dimensionless variables

$$\tau = \omega \sqrt{1 - f_2(T)} t, \quad v = w/a_0,$$

where  $a_0 = [\hbar/(m\sqrt{1 - f_2(T)}\omega)]^{1/2}$ , Eq. (11) becomes

$$v''(\tau) + v(\tau) = \frac{p}{v(\tau)^3}. \quad (12)$$

This equation, regarding  $v$  as the coordinate, describes the classical motion of a fictitious particle in the effective potential

$$V_{\text{eff}} = v^2 + p/v^2,$$

which admits an equilibrium point only when  $p > 0$ . In this case Eq. (12) has the analytical solution [19]

$$v^2(\tau) = \frac{1}{2} \left[ v_0^2 + \frac{p}{v_0^2} \pm \left( v_0^2 - \frac{p}{v_0^2} \right) \cos(2\tau) \right]. \quad (13)$$

The oscillation frequency is  $2\omega\sqrt{1 - f_2(T)}$ . For a two-dimensional harmonic trap,  $N_n \sim T^{5/2}$  [21–23], so the temperature dependency of the frequency is

$$\omega(T) \sim \sqrt{1 - CT^{1/2}},$$

where  $C$  is a constant independent of  $T$ . At zero temperature the frequency reduces to  $2\omega$ , as is expected. For a positive scattering length, the frequency decreases with increasing temperature. On the contrary, for a negative scattering length, the frequency increases with temperature. At a negative scattering length  $p$  becomes negative when  $N_0 > m^2/(2|a|\hbar^2)$ .

This gives a critical value of the atom number beyond which no condensate would occur, nor is there any oscillatory solution. This critical value is independent of the temperature.

In the case of a three-dimensional cylindrically symmetric harmonic trap

$$U(\mathbf{r}) = \frac{1}{2}m\omega^2(x^2 + y^2 + \lambda^2z^2), \quad (14)$$

the equations for the widths, in terms of the dimensionless constant  $P_0 = \sqrt{2/\pi}N_0(T)a/a_0$  and new dimensionless variables  $\tau = \omega t$ ,  $\nu_i = w_i/a_0$  with  $i = x, y, z$  and  $a_0 = \sqrt{\hbar/m\omega}$ , are

$$\frac{d^2\nu_x}{d\tau^2} + [1 - f_3(T)]\nu_x = \frac{1}{\nu_x^3} + \frac{P_0}{\nu_x^2\nu_y\nu_z}, \quad (15)$$

$$\frac{d^2\nu_y}{d\tau^2} + [1 - f_3(T)]\nu_y = \frac{1}{\nu_y^3} + \frac{P_0}{\nu_y^2\nu_x\nu_z}, \quad (16)$$

$$\frac{d^2\nu_z}{d\tau^2} + [\lambda^2 - f_3(T)]\nu_z = \frac{1}{\nu_z^3} + \frac{P_0}{\nu_z^2\nu_x\nu_y}. \quad (17)$$

Here, introducing the notation  $\eta = T/T_c$ ,  $\bar{\omega} = \lambda^{1/3}\omega$  and  $\bar{a}_0 = \sqrt{\hbar/m\bar{\omega}}$ , we have denoted for  $d = 3$

$$f_3(T) = f(T) = \eta^{\frac{5}{2}}N_n(T)\frac{a}{\bar{a}_0}\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\left[\frac{\zeta(3)}{N_0(T_c)}\right]^{\frac{5}{6}}.$$

The  $f_3(T)$  terms come from the interaction between the condensate and the thermal cloud. The  $\nu_i^{-3}$  terms correspond to the kinetic energy contribution which is neglected in the Thomas-Fermi approximation but plays a role in stabilizing the condensate. As in the case of zero temperature, for a positive scattering length  $a > 0$ , the effective potential has a stable equilibrium point, while for a negative scattering length  $a < 0$  there may be no equilibrium points, depending on  $N_0$  in comparison with a critical value  $N_c$ . For an attractive interatomic interaction,  $N_c$  sets an upper limit of the atom number, i.e. a collapse occurs when  $N_0 > N_c$ . When  $N_0 < N_c$ , a metastable equilibrium point exists as one of the two equilibrium points, supporting the condensate. In contrast to the two-dimensional case, for a three-dimensional trap, the critical atom number increases with temperature. This is consistent with what is known in the case of an isotropic trap [20].

Following Ref. [13], we may study the collective excitation modes of the condensate by expanding  $\nu_i$  of Eqs. (15)-(17) around the stable equilibrium point  $(\nu_0, \nu_0, \nu_{0z})$ , which satisfies

$$[1 - f_3(T)] \nu_0 = \frac{1}{\nu_0^3} + \frac{P_0}{\nu_0^3 \nu_{0z}}, \quad (18)$$

$$[\lambda^2 - f_3(T)] \nu_{0z} = \frac{1}{\nu_{0z}^3} + \frac{P_0}{\nu_0^2 \nu_{0z}^2}. \quad (19)$$

A linear analysis then leads to the following expressions for the low excitation frequencies

$$\omega(|m| = 2) = 2\omega\sqrt{1 - f_3(T) - 2P_{4,1}}, \quad (20)$$

$$\begin{aligned} \omega(|m| = 0) &= \sqrt{2}\omega \left[ (1 - f_3(T)) (1 + \lambda^2(T)) - P_{2,3} \right. \\ &\quad \left. \pm \sqrt{[(1 - f_3(T)) (1 - \lambda^2(T)) + P_{2,3}]^2 + 8P_{3,2}^2} \right]^{\frac{1}{2}}, \end{aligned} \quad (21)$$

where  $P_{i,j} = P_0/(4\nu_0^i \nu_{0z}^j)$  and  $\lambda^2(T) = (\lambda^2 - f_3(T))/(1 - f_3(T))$ , and we have labeled the modes by the azimuthal angular quantum numbers  $m$ . By noticing that  $f_3(T) = 0$  at zero temperature, expressions (20) and (21) reproduce the results obtained in Ref. [13].

For small  $P_0$ , expressions (20) and (21) are close to the bare trap results. For large values of  $P_0$  they correspond to the case of large interatomic interactions in comparison with the trap excitation energies. They are good for either the repulsive or attractive interatomic interactions, i.e. for both the positive and negative scattering lengths. In the large atom number limit, where the kinetic energy term is negligible, expressions (20) and (21) can be further simplified as

$$\omega(|m| = 2) = \omega\sqrt{2(1 - f_3(T))}, \quad (22)$$

$$\omega(|m| = 0) = \omega\sqrt{\frac{1 - f_3(T)}{2}} \left[ 4 + 3\lambda^2(T) \pm \sqrt{16 + 9\lambda^4(T) - 16\lambda^2(T)} \right], \quad (23)$$

which, with  $(1 - f_3(t))\omega$  replaced by  $\omega$  and  $(\lambda^2 - f_3(t))/(1 - f_3(T))$  by  $\lambda^2$  at zero temperature, correspond to the Thomas-Fermi approximation. Near the critical temperature  $N_0$  is small, so the interatomic interaction of the condensate may not be dominant over the kinetic energy. For attractive interacting Bose gases of a negative scattering length, no condensate exists without the contribution of the kinetic energy being included. In these cases, instead of expressions (22) and (23), expressions (20) and (21) should be used.

In the MIT experiment [7], the axial trapping frequency  $\nu_z = 16.93\text{Hz}$  and the radial frequency  $\nu_r = 230\text{Hz}$ . Without considering the interatomic interaction, the critical tem-

perature  $kT_c = \hbar\omega(N\lambda/1.202)^{1/3}$  [21–23] for  $N = 80 \times 10^6$  is  $1.87\mu\text{K}$ , which is close to the experimental value  $T_c = 1.7\mu\text{K}$ . The difference may come from the neglected atomic mutual interaction [23,24]. According to the local density approximation the chemical potential is given by [25]

$$\mu = \frac{8\pi a\rho_0\hbar^2}{m} + \frac{\hbar\bar{\omega}}{2} \left\{ \frac{15aN}{\bar{a}_0} \left[ 1 - \left( \frac{T}{T_c} \right)^3 \right] \right\}^{\frac{2}{5}}, \quad (24)$$

which, for very low temperatures, reduces to

$$\mu = \frac{\hbar\bar{\omega}}{2} \left[ \frac{15aN}{\bar{a}_0} \right]^{\frac{2}{5}}.$$

Noticing that  $a = 2.75\text{nm}$  in the MIT experiment, we have the chemical potential  $\mu/k_B \approx 348\text{nK}$  at  $N_0 = 15 \times 10^6$  in agreement with the experimental value  $380\text{nK}$ . This verifies the validity of the local density approximation.

Using the experimental parameters we have calculated the oscillation frequencies. For the experiment on Rb vapor at JILA, the particle number is not too large, so expressions (20) and (21) are used. The temperature dependent excitation spectrum from the theoretical calculation together with the experimental measurements is shown in Fig. 1. It is seen that at low temperatures the frequencies decrease with increasing temperature. A simple theory explains the experimental data at low temperature when the condensate occupies a significant proportion. In the MIT experiment for mode  $m = 0$ , the atom number is rather large, so we use expressions (22) and (23). The comparison of the theory with experiment is shown in Fig. 2. The theoretical results are in good agreement with experimental observation.

In summary, by including a mean field acting on the condensate from the static thermal cloud in the Lagrangian density, we have studied the collective excitation modes of BEC at finite temperature by means of the time-dependent variational method, and obtained analytic expressions for the temperature-dependent frequency shift of low excitation modes. We have compared the theory with experimental observations. The theoretical results are in agreement with the MIT experiment very well.

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## FIGURES

FIG. 1. Temperature-dependent excitation spectrum of the JILA experiment for collective modes  $m = 0$  (triangle) and  $m = 2$  (circle), compared with theoretical curves (dotted for  $m = 0$  and solid for  $m = 2$ ). Frequencies are normalized with respect to the radial trap frequency, and temperature to the critical temperature for a harmonically confined ideal gas

FIG. 2. Temperature-dependent collective excitation frequencies of the MIT experiment for mode  $m = 0$  (circle), compared with the theoretical curve. In the experiment, temperature was varied by adjusting the rf frequency of a magnetic trap, so here  $\Delta\nu_{\text{rf}}$  is a measure of temperature.



